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Composite Reinforcement using Boron Nitride Nanotubes

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THE UNIVERSITY OF QUEENSLAND

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14. ABSTRACT
Boron nitride nanotubes (BNNTs) have been proposed as a suitable reinforcement for metal matrix composites resulting in materials high mechanical strength. In this work quantum chemical calculations have been carried out to examine the strength of interactions of metals with BNNTs in order to provide insight into their bonding. Calculations were also carried out to study the effect of oxygen on the interactions. Titanium and aluminium are considered due to their relatively low densities, and copper is considered because copper alloys are known to have desirable properties for use as a structural material. Metal atoms, tetra-atomic metal clusters and metal surfaces comprising Al, Ti and Cu are considered, in addition to different crystal faces of an Al slab. Effects including the chirality of the nanotube, its diameter and the influence of vacancy defects and doping with carbon (producing boron/carbon nitride nanotubes, BCNNTs) have been studied.

Ti exhibits the strongest binding to the BNNTs regardless of the conditions (impurities, defects or size of the cluster) and that C sites on the BCNNTs significantly increase the binding of the metals to the BNNTs. Among the three metals studied, Al is most sensitive to changes in the tube size, imperfections or defects in its atomistic environment, which often results in notable changes of its binding to the system. By contrast, Cu and Ti exhibits quite uniform behaviour and hardly change their binding energy with tube size for the systems investigated.

Studies on the interaction of BNNTs with the surfaces of metal slabs found similar results with the main conclusions. Studies on how the interactions present at the interface of small aluminium clusters and boron nitride nanotubes change with the presence of atomic oxygen were also carried out.

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4. Organization: The Australian Institute for Bioengineering and Nanotechnology, The University of Queensland

5. Research Team: Debra J. Bernhardt (Project PI), Christoph Rohmann (Postdoctoral Research Fellow employed using project funds), Jack Rainey (4th Year Honours Student)

6. Summary: Boron nitride nanotubes (BNNTs) have been proposed as a suitable reinforcement for metal matrix composites resulting in materials high mechanical strength. In this work quantum chemical calculations have been carried out to examine the strength of interactions of metals with BNNTs in order to provide insight into their bonding. Calculations were also carried out to study the effect of oxygen on the interactions. In this project titanium and aluminium are considered due to their relatively low densities, and copper is considered because copper alloys are known to have desirable properties for use as a structural material. Metal atoms, tetra-atomic metal clusters and metal surfaces comprising Al, Ti and Cu are considered, in addition to different crystal faces of an Al slab. Effects including the chirality of the nanotube, its diameter and the influence of vacancy defects and doping with carbon (producing boron/carbon nitride nanotubes, BCNNTs) have been studied.

It was found that titanium exhibits the strongest binding to the BNNTs regardless of the conditions (impurities, defects or size of the cluster) and that C sites on the BCNNTs significantly increase the binding of the metals to the BNNTs. Among the three metals studied, we find that Al is most sensitive to changes in the tube size, imperfections or defects in its atomistic environment, which often results in notable changes of its binding to the system. By contrast, Cu and Ti exhibits quite uniform behaviour and hardly change their binding energy with tube size for the systems investigated.

Studies on the interaction of BNNTs with the surfaces of metal slabs found similar results with the main conclusions being that Al binds relatively weakly unless there is a B vacancy in the BNNT. In that case the binding energy increases to be similar to that of a Ti surface with a pristine BNNT. In the case that there is a B vacancy, an aluminium atom becomes bound to the BNNT surface might be the origin of AlN and AlB_2 species. Ti binds strongly in all cases and Cu has surprisingly strong bonded, although the higher density of Cu would suggest that it would be most promising in an alloy.

Studies on how the interactions present at the interface of small aluminium clusters and boron nitride nanotubes change with the presence of atomic oxygen were also carried out. It was found that with a low concentration of oxygen, formation of Al_4O_x clusters was preferred over

interactions of the oxygen with the nanotube. These then bind to the nanotube weakly to the BNNT with van der Waals forces. A further increase of oxygen in the system results in the aluminium cluster being oxidised and distorted, binding to the nanotube through chains of AlO. It was also found that oxygen chemisorbed on the nanotube can be extracted via the addition of pure aluminium, which is bound to the metal cluster as well as the BNNT, resulting in a strong binding interface.

7. Background:

New strong, lightweight and cost-effective materials are required for a wide range of applications including the aerospace, transport and defence industries. Use of nanotubes for reinforcement of metal matrix composites has shown much promise, yet there is a demand for improvement, especially with regard to the integrity of the metal matrix composite and its chemical stability. In addition, potential issues that would cause fabrication difficulties need to be considered. The fundamental understanding of interactions between the reinforcement and the metal matrix is essential, as is the effect of the presence of oxygen. In this project quantum chemical calculations are being used to provide the knowledge to develop this understanding. The research team collaborates with experimental experts in the field to ensure that the computational research is directed towards addressing practical issues.

Boron nitride nanotubes have been proposed as a suitable reinforcement for metal matrix composites. In order to be effective, the interaction between the metal and the nanotube needs to be strong while retaining the nanotube structure. As part of a previous project (AOARD Grant 134071), calculations were carried out to study the interactions of boron nitride nanotubes (BNNTs) with aluminium (Al) and titanium (Ti) atoms and small clusters. These metals were introduced as single atoms, small clusters consisting and preliminary results have been obtained on metal surfaces. Furthermore pristine BNNT, BNNT with boron (B) or nitrogen (N) defective sites and BNNTs with C doping were considered. This work has been continued as part of the current project. However, in addition to Al and Ti, in this project Cu will be considered. This is because preliminary experimental work indicated that BNNT reinforced Cu is rather brittle and therefore comparison of the behaviour of Al, Ti and Cu is important, and also because Cu is used in alloys to produce materials of high mechanical strength.

Although it is useful to obtain results for interaction of single metal atoms and clusters, interaction with metal surfaces will be more representative of the real system. Therefore this project aims to look at the interaction of metals surfaces with pristine and defective BNNTs, and BNNTs doped with carbon atoms. Due to their potential, various surfaces of an aluminium slab were considered. Again the dependence on pore radius and chirality were investigated.

In addition to the strength of the interaction between the metal and BNNT, there are other issues that need to be addressed when fabrication of the metal matrix composite material is considered. There are various approaches to fabrication, and in some processes high temperature reaction products that might be produced. This means that it will be useful to computationally determine the stability of potential reaction products and the strength of interactions between these products and the BNNT. If there is significant reaction between the metal and the BNNT, we propose that it might be necessary to use multi-walled nanotubes in order to maintain the integrity of the reinforcing material.

In fabrication, the presence of oxygen is also of importance. If it is necessary to apply strict control of oxygen in the atmosphere, fabrication will often require more complex and costly processes. In commercial production, the production of Al alloys using powder metallurgy involves sintering in high purity N_2 atmosphere to prevent formation of oxides on the powder. The presence of residual oxygen in the sintering atmosphere is the key reason for the problems of surface porosity and distortion of the alloys produced. [1] In addition, there is a surface oxide film on each Al powder particle which, in industrial production, is disrupted by the addition of about 0.5–1.5 wt % Mg powder during sintering in order to enable effective interfacial bonding between the Al powder particles at low fabrication temperatures. The formation of BNNT reinforced Al might require similar conditions and rigorous control of oxygen might be necessary, and the effect of oxygen will therefore be considered in this project.

8. Methodology:

Quantum chemical density functional theory calculations were used to investigate the utility of BNNTs as a reinforcement material in metal matrix composites. Pristine and defective nanotubes of various radius, and clusters of 1-4 atoms of Al or titanium (Ti) atoms were considered in our previous project (AOARD Grant 134071). Studies on the interaction of the BNNTs with indices from (5,5) to (10,10) were considered. However during early stages of the current project it was found that spin polarization, which had been neglected in the earlier work, had a large effect on some of the results. Therefore these calculations were repeated with spin-polarization allowed. Although the general trends remained in most cases, the quantitative results differed.

In this project, as well as Al and Ti, Cu is being considered. Periodic BNNTs or M@BNNTs (metal adsorbed on a BNNT) were studied with the supercell oriented so that the axis of the BNNT lies along the z-axis. Spin-polarized DFT calculations were performed as implemented in the Vienna Ab initio Simulation Package (VASP) [2] for all calculations. The Perdew−Burke−Ernzerhof (PBE) functional within the generalized gradient approximation (GGA) approach was employed to model the exchange correlations. [3] The ion−electron interaction is described by ultra soft pseudo potentials. [4] All structures were fully relaxed until the total energy converged to 1.0×10^{-4} eV within the self-consistent loop and forces of less than 0.01 eV/Å were reached. The k-space was sampled with a 1 × 1 × 1 Monkhorst−Pack mesh, [5] and an energy cutoff of 400 eV was used for all calculations. van der Waals interactions were accounted for by means of the Grimme scheme. [6] Density of state (DOS) calculations were carried out with a 1 × 1 × 12 Monkhorst−Pack mesh.

Initial test calculations were conducted to determine the appropriate energy cutoff and number of k-points, with results showing less than 0.01 eV changes in the binding energy upon an increase to 450 eV or a k-point mesh of 1×1×6. Prior to creating the supercells, the dimensions of each NT were optimized with respect to the c lattice constant (the axis of the NT), while a vacuum layer of at least 15 Å was added in the a and b directions. To model the clean and adsorbate-covered structures, 1 × 1 × 5 supercells were considered for the armchair NTs, and 1 × 1 × 3 supercells for the zigzag BNNTs. A single unit cell was sufficient for the (10,5) and (9,6) NTs due to their length. A minimum value of 11.5 Å for c (15 Å for a and b) was used to ensure that the interaction of the adsorbed species with its periodic image is small.

The binding energy, E_b, was determined from the difference in the energy of the metal

cluster bound to the nanotube, $E_{M_n\text{-}BNNT}$, and the nanotube, E_{BNNT}, and cluster energy, E_{M_n}:

$$E_b = E_{M_n\text{-}BNNT} - (E_{BNNT} + E_{M_n}) \quad (1)$$

where M is either Al or Ti and n is the number of atoms in the cluster. This process was then repeated with one B or one N atom removed from the BNNT unit to give a defective nanotube, or with a carbon atom replacing one of the boron or nitrogen atoms.

In addition to this, calculations on the interaction of BNNTs with an metals surface were carried out by constructing models of the most common surfaces: an Al [100], [110] and [111] surfaces, Ti [0,1,1] and [1,1,1] surfaces, and Cu [1,1,0] and [1,1,1] surfaces. These comprised a periodic slab with a thickness of up to 7 atoms. The behaviour of the binding energy and structures formed were examined.

To examine the effect of oxygen at the interfaces between a metal and a nanotube, calculations have been designed to consider the interaction of atomic oxygen with pre-formed Al@BNNT, the interaction of preformed aluminium oxides (Al_4O_x) with a pristine and oxidised BNNT, and the interaction of pure Al_4 clusters with an oxidised BNTT.

9. Results and Discussion:

Figure 1 shows how the binding energy changes with the diameter of the BNNT and the metal atom considered.

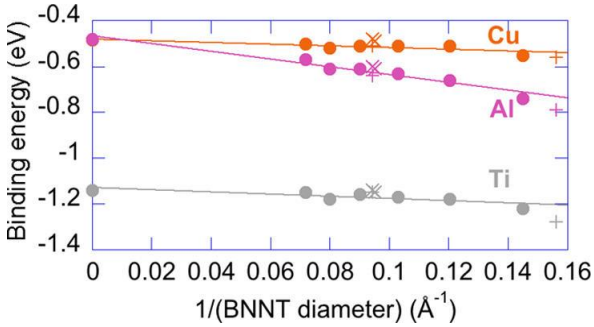

Figure 1. Variation of the binding energies of Ti, Al, and Cu to pristine BNNTs as a function of the inverse diameter of the nanotube. Results for armchair (●), zigzag (+), and chiral (×) nanotubes are shown. The lines are a guide to the eye.

The binding energy varies as approximately 1/d, where d is the diameter of the BNNT, apart from very small diameters. However it is clear that if strong binding is desired, decreasing the diameter of the BNNT can help. Our results show that the smallest nanotube considered (the (8,0) BNNT) exhibits a significantly different binding energy and adsorption geometry in all cases investigated compared to larger diameter BNNTs considered here. Therefore, this suggests that, once the diameter of the tube is less than a critical value, the behavior will change. In contrast, our data show that the interaction of Al, Ti, and Cu with h-BN sheets is comparable to that of the BNNTs with the largest diameter considered, with the exception of those systems where the adsorption takes place at a N vacancy. Therefore, h-BN sheets provide good models of BNNTs, provided they are not too small.

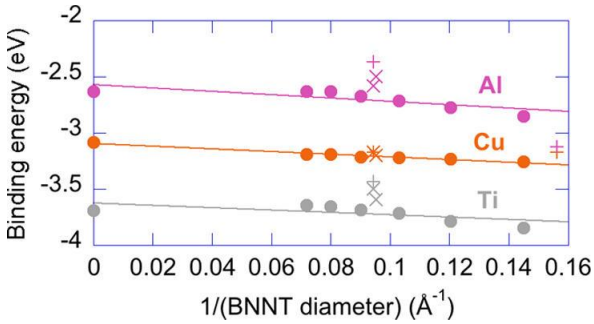

Figure 2. Variation of the binding energies of Al, Ti, and Cu to BNNTs with an N vacancy as a function of the inverse diameter of the nanotube. Results for armchair (●), zigzag (+), and chiral (×) nanotubes are shown. The result for the smallest diameter nanotube, (8,0), is not shown for Ti as this binding energy is much larger than the others shown in this figure (−6.10 eV). The lines are a guide to the eye.

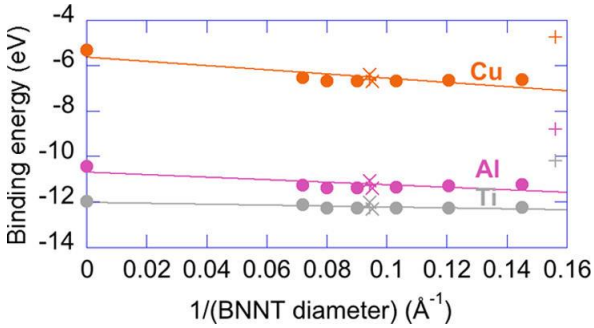

Figure 3. Variation of the binding energies of Ti, Al, and Cu to BNNTs with a B vacancy defect as a function of the inverse diameter of the nanotube. Results for armchair (●), zigzag (+), and chiral (×) nanotubes are shown. The lines are a guide to the eye.

Similar trends were obtained when vacancy defects appeared in the BNNT, as shown in Figures 2 and 3, however in the case of an N vacancy defect the chirality played an important role. The effects on the binding energy of C substitutions are also shown in Figure 4. Vacancies (N or B) and C substitutions strongly enhance the binding of Al, Ti, and Cu. Our results show that the adsorption taking place at a B vacancy results in a significantly stronger binding of the metal to the BNNT than to a CNT (with or without a C vacancy) of similar diameter.

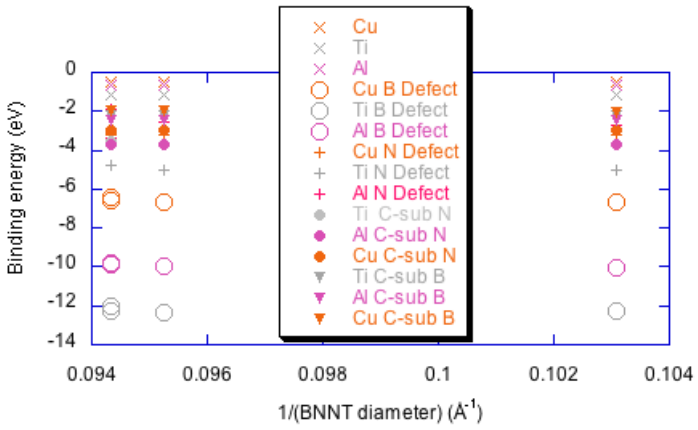

Figure 4. Summary of results for binding of single metal atoms on BNNTs of varying diameter.

This work is has been published in "Interaction of Al, Ti, and Cu Atoms with Boron Nitride Nanotubes: A Computational Investigation" by Christoph Rohmann, Qiao Sun, and Debra J. Searles (Bernhardt) in the Journal of Physical Chemistry C [7].

In our initial studies on the interaction between metal surfaces and BNNTs, a (7,7) BNNT and the [100] surface of an aluminium slab was considered. We considered the changes in binding energy and structure with the number of Al atom layers, and these are presented in Figure 5. Although convergence is rather erratic, the changes in binding energy with change in the number of layers is small compared to the changes with the structure of the BNNT. In addition the trends are similar to those observed for the single atom. This is because the strong interactions generally involve interaction of one metal atom from the slab with the BNNT, with the additional energy being due to weak interactions of the pristine systems. The computational expense of the calculations for the slabs are orders of magnitude larger than those for the single atom, and therefore these results suggest that preliminary calculations with the single atom are very worthwhile in any computational study.

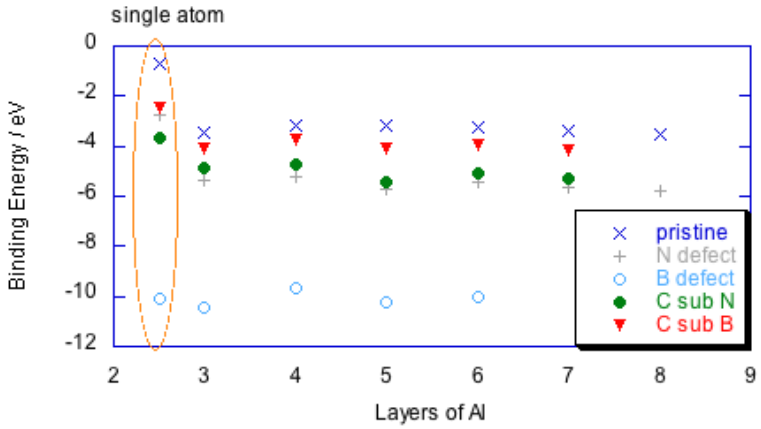

Figure 5. Variation in binding energy of various (7,7) BNNTs to aluminium slabs as a function of the number of the number of layers of atoms in the slabs. The circled points are the binding energies for single atoms with the different nanotubes.

The binding energies obtained for the various surfaces are presented in Table 1. The binding energies between Ti and the BNNTs are the highest in all cases, with the surface considered making a significant difference for the pristine nanotube. Weakest binding is observed for Al, although that is also strong binding when the BNNT has a B vacancy. Figure 6 shows how the surface and the BNNT interact, and figure 6b it can be since that an Al atom has moved close to the vacancy left by the B atom. It is also to be noted that the Ti nanotubes, which are all very strongly bound to the surface, are quite distorted. This could have implications for their electronic properties that would be worth further investigation. Quite strong bonding is observed for the all the BNNTs to all the Cu metal surfaces, and interestingly the structure of the surface does not appear to be altered very much by the presence of the BNNT.

Table 1. Binding energies (eV) for various nanotubes on Al, Ti and Cu surfaces.

	Al[100] Surface	Al[110] Surface	Al[111] Surface	Ti[111] Surface	Ti[011] Surface	Cu[110] Surface	Cu[111] Surface
Pristine	-0.41	-0.46	-0.48	-1.77	-2.33	-0.95	-0.90
Single Atoms/ Cluster	-0.63/-0.34			-1.17/-1.44		-0.51/-0.65	
N-Defect	-0.69	-0.71	-0.56	-2.00	-2.71	-1.23	-1.33
B-Defect	-1.26	-1.64	-1.21	-3.30	-3.69	-1.97	-1.73
C$_N$	-0.64	-0.77	-0.71	-2.17	-2.70	-1.26	-1.22
C$_B$	-0.51	-0.56	-0.53	-1.41	-2.50	-1.00	-1.01
Repeat Units	8	8	9	6	7	6	6

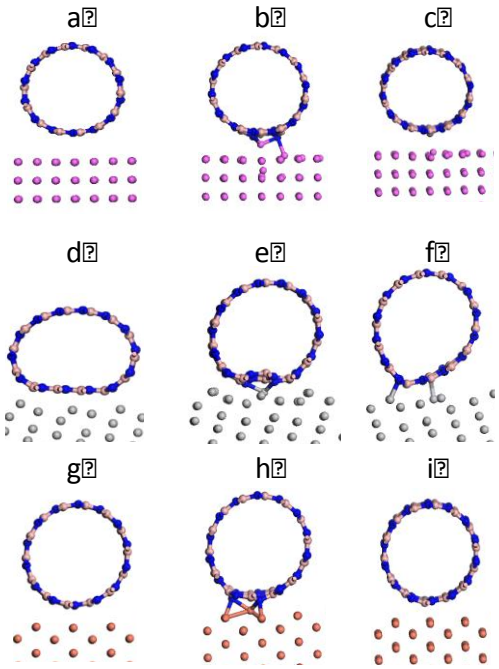

Figure 6. Interaction of BNNTs with Al [110] (a-c), Ti [111] (d-f) and Cu [110] (g-i) surfaces. Pristine BNNTs were considered in the first column (a,d,g), BNNTs with a B vacancy in the second column (b,e,h) and C-doped BNNTs with a C atom replacing a B atom in the third column (c, f, i).

Further study was carried out on the various Al surfaces, and the change in charge density was calculated to provide information on the type of bonding occurring between the BNNT and the metal. An increase in the charge density is evidence of formation of a bond. Some results are presented in Figure 7 and this shows that there is significant bonding between the BNNT and surface when the BNNT has a B vacancy and if a C atom replaces a B atom. This is considerable contrast with the pristine BNNT where there is little change in charge density. This gives insight into the behavior observed in fabrication where in some cases This work is being prepared for publication with collaborators met through the support provided by this project, from (NASA) and Dr Vesselin Yamakov (National Institute of Aerospace - NIA).

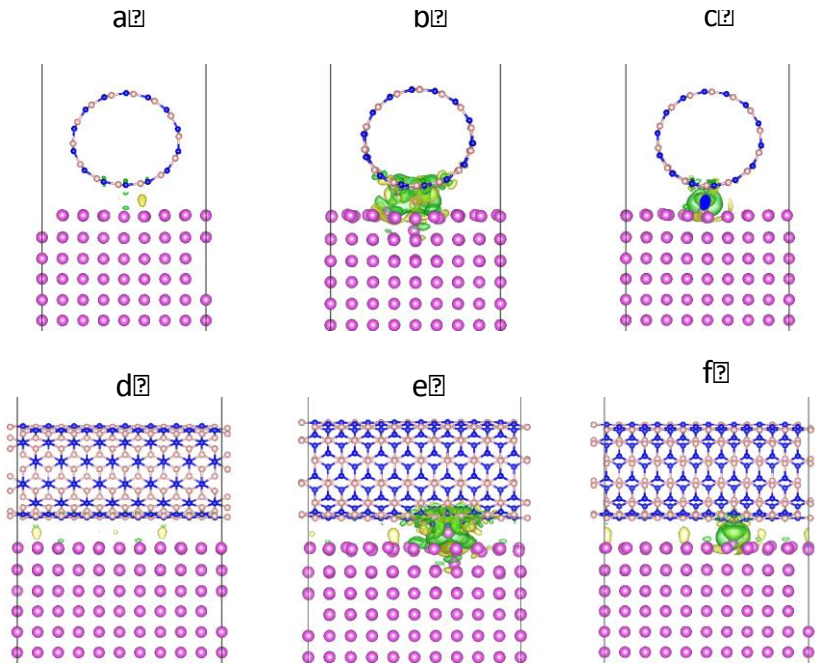

Figure 7. Two views of the change in charge density due to interaction of an Al [110] surfaces with a pristine BNNT (a) and (d), BNNT with a B vacancy (b) and (e) and C-doped BNNT with a C atom replacing a B atom (c) and (f).

Calculations on the effect of oxygen at the interface between the metal atoms and BNNTs was studied using various possibilities for the type of interaction. The interaction of atomic oxygen with a pre-formed Al-BNNT, the interaction of aluminium oxides (Al_4O_x) with a pristine and oxidized BNNT, and the interaction of pure Al_4 clusters with an oxidized BNNT were considered. This work was part of a 4th year student research project (Honours project) for 2016 by Jack Rainey. He received a 1st Class Honours degree for his work.

10. Ongoing work

The work on binding between the Al metal surfaces and BNNTs is in preparation for publication. A first draft has been completed and is being considered by our collaborators at NASA/NIA.
In addition to this work, the work comparing Al, Ti and Cu surface interactions will be

prepared for publication. This work will also be presented at PacSurf 2016 in Hawaii, December 2016, presented by John-Andrew Hocker from NASA (see [8]).

11. References:

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8. John-Andrew Hocker, *NASA Langley Research Center*, USA*;* S-H. Chu, V. Yamakov, *National Institute of Aerospace, USA;* J. Newman, S. Messina, E. Judd, *NASA Langley Research Center, USA;* C. Rohmann, D. Bernhardt, *The University of Queensland, Australia;* C. Park, C. Fay, *NASA Langley Research Center, USA*; **Boron Nitride Nanotube-Titanium Alloy Nanocomposites**, abstracts available http://www.avsconferences.org/PacSurf/.

12. Publications and presentations resulting from the project:

1. John-Andrew Hocker, *NASA Langley Research Center*, USA*;* S-H. Chu, V. Yamakov, *National Institute of Aerospace, USA;* J. Newman, S. Messina, E. Judd, *NASA Langley Research Center, USA;* C. Rohmann, D. Bernhardt, *The University of Queensland, Australia;* C. Park, C. Fay, *NASA Langley Research Center, USA*; **Boron Nitride Nanotube-Titanium Alloy Nanocomposites**, abstracts available http://www.avsconferences.org/PacSurf/ (oral presentation to be give by John-Andrew Hocker)

2. Annual Science Conference of China-Australia Joint Laboratory for Energy & Environmental Materials; 8-10 Nov. 2015, Guangzhou, China "Computational studies on materials for energy applications" (oral presentation by Debra J Searles)

3. NIA and NASA talk, Friday, May 8, 2015, Hampton, VA, USA, "Computational modelling of materials and fluids on the molecular level" (http://nia-mediasite.nianet.org/NIAMediasite100/Play/c2d8f3660e8641458163a9f379ac16fa1d) (oral presentation by Debra J. Searles)

4. AFRL, Wright-Patterson Air Force Base, Dayton, OH, USA, May 4, 2015 "Non-Equilibrium Simulations: Property Predictions using Novel Computational Approaches" (oral presentation by Debra J. Searles)

5. AFOSR talk, May 7, 2015 Low Density Materials Program talk, Arlington, VA, USA "Composite Reinforcement Using Boron Nitride Nanotubes" (oral presentation by Debra J. Searles)

6. NIA and NASA, Hampton, VA, USA, December 12, 2014, "Computational Studies Towards Metal Matrix Composite Reinforcement using Boron Nitride Nanotubes" (oral

presentation by Christoph Rohmann)

7. Molecular Modelling, 30 of July – 2nd of August, 2014, Gold Coast, Australia, "Composite Reinforcement Using Boron Nitride Nanotubes“ (poster presentation by Christoph Rohmann)

13. Significant collaborations resulting from the project:

1. ***Collaboration with NASA and NIA***: This work has led to a collaboration with Dr Cheol Park from (NASA) and Dr Vesselin Yamakov (National Institute of Aerospace - NIA), experimental experts in the synthesis of BNNTs and their characterisation. This collaboration was initiated during the AFOSR 2014 Low Density Materials Program Review in June 2014.
Christoph Rohmann made an extended visit to NIA and NASA LaRC, January – March 2015 and Debra Bernhardt visited NIA and NASA and presented a seminar on 8 May 2015.

2. ***Interaction with AFRL****:* Debra Bernhardt visited AFRL, Wright-Patterson Air Force Base, Dayton, OH, USA, May 4, 2015. A formal collaboration with Dr Rajiv Berry is being developed with two projects of current interest: “Selective Sequestration of Multi-Component Compounds using Engineered Gas Vesicles” and “Design of Polymers for Additive 3D Printing via Non-Equilibrium Molecular Dynamics”.

3. ***AFOSR 2015 Low Density Materials Program Review***: Debra Bernhardt presented her work at this meeting.

14. Additional support for project:

Visits to NASA LaRC, Wright-Patterson Air Force Base and AFOSR Program review were supported by a WOS award.
Support for Christoph Rohmann’s extended visit to NIA and NASA was supported by funding from The University of Queensland.
Extensive computing time was required for this work and was obtained with the support of The University of Queensland’s allocation of time as part of an Australian Research Council LIEF grant as well as access to facilities at NIA/NASA.